

$\bar{4}2cm$

$4mm$

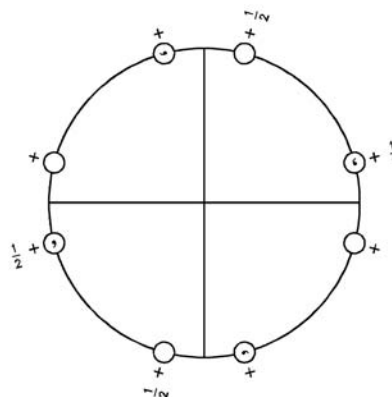
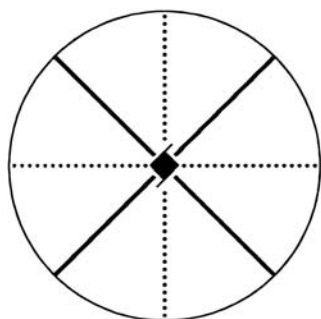
Tetragonal

No. 35

$\bar{4}2cm$

Patterson symmetry  $\bar{4}4/mmm$

FIRST SETTING



**Origin** on  $2mm$  on  $4_2cm$

**Asymmetric unit**  $0 \leq x; 0 \leq y; 0 \leq z \leq 1; x \leq y$

**Symmetry operations**

- |  |  |   |   |
|--|--|---|---|
| (1) 1<br>(1 0,0,0)                               | (2) $2_{z^2}$ 0,0,z<br>( $2_z$  0,0,0)           | (3) $4^+(\frac{1}{2})$ 0,0,z<br>( $4_z^+$  0,0, $\frac{1}{2}$ ) | (4) $4^-(\frac{1}{2})$ 0,0,z<br>( $4_z^-$  0,0, $\frac{1}{2}$ ) |
| (5) $c_x$ x,0,z<br>( $m_y$  0,0, $\frac{1}{2}$ ) | (6) $c_y$ 0,y,z<br>( $m_x$  0,0, $\frac{1}{2}$ ) | (7) $m_{xz}$ x, $\bar{x}$ ,z<br>( $m_{xy}$  0,0,0)              | (8) $m_{yz}$ x,x,z<br>( $m_{xy}$  0,0,0)                        |

**Generators selected** (1);  $t(0,0,1)$ ; (2); (3); (5)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 <i>c</i> 1	(1) $x, y, z$ (5) $x, \bar{y}, z + \frac{1}{2}$	(2) $\bar{x}, \bar{y}, z$ (6) $\bar{x}, y, z + \frac{1}{2}$	(3) $\bar{y}, x, z + \frac{1}{2}$ (7) $\bar{y}, \bar{x}, z$	(4) $y, \bar{x}, z + \frac{1}{2}$ (8) $y, x, z$	$l : l = 2n$  Special: no extra conditions
4 <i>b</i> $\dots m$	$x, x, z$	$\bar{x}, \bar{x}, z$	$\bar{x}, x, z + \frac{1}{2}$	$x, \bar{x}, z + \frac{1}{2}$	
2 <i>a</i> $2 \dots mm$	$0, 0, z$	$0, 0, z + \frac{1}{2}$			

**Symmetry of special projections**

Along [001] $4mm$	Along [100] $\mu 11m$	Along [110] $\mu 11m$
Origin at $0, 0, z$	$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ Origin at $x, 0, 0$	$\mathbf{a}' = \mathbf{c}$ Origin at $x, x, 0$

**Maximal non-isotypic non-enantiomorphic subgroups**

<b>I</b>	$[2] \mu 4_2 11 (\mu 4_2, 25)$	1; 2; 3; 4
	$[2] \mu 2c1 (\mu cc2, 16)$	1; 2; 5; 6
	$[2] \mu 21m (\mu mm2, 15)$	1; 2; 7; 8

**IIa** none

**IIb** none

**Maximal isotypic subgroups and enantiomorphic subgroups of lowest index**

**IIc**  $[3] \mu 4_2 cm (\mathbf{c}' = 3\mathbf{c}) (35)$

**Minimal non-isotypic non-enantiomorphic supergroups**

**I**  $[2] \mu 4_2 / mmc (41)$

**II**  $[2] \mu 4mm (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (34)$

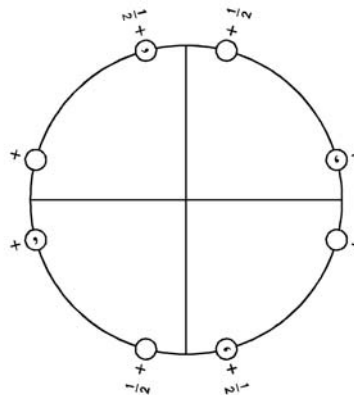
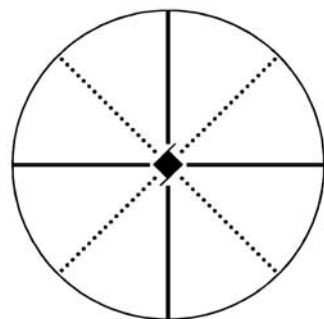
$\bar{4}2m$  $4mm$ 

Tetragonal

No. 35

 $\bar{4}2m$ Patterson symmetry  $\bar{4}2m$ 

## SECOND SETTING

**Origin** on  $2mm$  on  $4_2mc$ **Asymmetric unit**  $0 \leq x; 0 \leq y; 0 \leq z \leq 1; x \leq y$ **Symmetry operations**

- |                                    |                                    |   |  |
|------------------------------------|------------------------------------|---|--|
| (1) 1<br>(1 0,0,0)                 | (2) 2 $0,0,z$<br>( $2_z$  0,0,0)   | (3) $4^+(\frac{1}{2})$ $0,0,z$<br>( $4_z$  0,0, $\frac{1}{2}$ ) | (4) $4^-(\frac{1}{2})$ $0,0,z$<br>( $4_z^{-1}$  0,0, $\frac{1}{2}$ ) |
| (5) $m$ $x,0,z$<br>( $m_y$  0,0,0) | (6) $m$ $0,y,z$<br>( $m_x$  0,0,0) | (7) $c$ $x,\bar{x},z$<br>( $m_{xy}$  0,0, $\frac{1}{2}$ )       | (8) $c$ $x,x,z$<br>( $m_{xy}$  0,0, $\frac{1}{2}$ )                  |

**Generators selected** (1);  $t(0,0,1)$ ; (2); (3); (5)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 <i>c</i> 1	(1) $x, y, z$ (5) $x, \bar{y}, z$	(2) $\bar{x}, \bar{y}, z$ (6) $\bar{x}, y, z$	(3) $\bar{y}, x, z + \frac{1}{2}$ (7) $\bar{y}, \bar{x}, z + \frac{1}{2}$	(4) $y, \bar{x}, z + \frac{1}{2}$ (8) $y, x, z + \frac{1}{2}$	$l : l = 2n$
4 <i>b</i> . <i>m</i> .	$x, 0, z$	$\bar{x}, 0, z$	$0, x, z + \frac{1}{2}$	$0, \bar{x}, z + \frac{1}{2}$	Special: no extra conditions
2 <i>a</i> 2 <i>mm</i> .	$0, 0, z$	$0, 0, z + \frac{1}{2}$			

**Symmetry of special projections**

Along [001] $4mm$	Along [100] $\mu 11m$	Along [110] $\mu 11m$
Origin at $0, 0, z$	$\mathbf{a}' = \mathbf{c}$ Origin at $x, 0, 0$	$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ Origin at $x, x, 0$

**Maximal non-isotypic non-enantiomorphic subgroups**

<b>I</b>	$[2]\mu 4_2 11 (\mu 4_2, 25)$	1; 2; 3; 4
	$[2]\mu 21c (\mu cc2, 16)$	1; 2; 7; 8
	$[2]\mu 2m1 (\mu mm2, 15)$	1; 2; 5; 6

**IIa** none

**IIb** none

**Maximal isotypic subgroups and enantiomorphic subgroups of lowest index**

**IIc**  $[3]\mu 4_2 mc (\mathbf{c}' = 3\mathbf{c}) (\mu 4_2 cm, 35)$

**Minimal non-isotypic non-enantiomorphic supergroups**

**I**  $[2]\mu 4_2 / m m c (41)$

**II**  $[2]\mu 4 m m (\mathbf{c}' = \frac{1}{2}\mathbf{c}) (34)$